

3«alpha»-Methylitaconyloxytropane

Inchi: InChI=1S/C14H21NO4/c1-9(6-13(16)18-3)14(17)19-12-7-10-4-5-11(8-12)15(10)2/h10-12
InchiKey: ITUZICAGZROVSJ-GDNZZTSVSA-N
Formula: C14H21NO4
SMILES: C=C(CC(=O)OC)C(=O)OC1CC2CCC(C1)N2C
Mol. weight [g/mol]: 267.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.96		Crippen Method
logp	1.274		Crippen Method
mcvol	206.960	ml/mol	McGowan Method
rinpol	1891.00		NIST Webbook
rinpol	1893.00		NIST Webbook
rinpol	1893.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R570060&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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